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Phase Transitions in Tricalcium Silicate

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Beamline(s): X7A

Introduction: Tricalcium silicate is the main component of cement clinker. The pure form exhibits phase transitions during heating, and goes through three triclinic and three monoclinic modifications before assuming rhombohedral symmetry, as follows [1]: $T_1 \rightarrow T_2 \rightarrow T_3 \rightarrow M_1 \rightarrow M_2 \rightarrow M_3 \rightarrow R$. The only forms to have fully determined structures are the T_1 [2], M_3 [3,4] and R [5,6] modifications, although the forms likely to be present in clinker are the M_3, M_1 and T_2 modifications [1]. Structural differences within the same space group are believed to involve shifts in the atomic positions of some atoms. Rietveld analysis is being used increasingly for the phase quantification of components in cement clinker, however the tricalcium silicate forms being modelled show deviations form those found in clinker [7]. As a result, the quantification of the total amount of tricalcium silicate is consistent, but the amount of each polymorph is highly variable. It is also possible that the polymorphs of tricalcium silicate being modelled in a Rietveld fit will compensate for those phases not being modelled and could lead to errors in the model, potentially for all phases concerned. A link between tricalcium silicate polymorphism and strength of cement has also been demonstrated [8].

Methods and Materials: Synchrotron diffraction data was gathered during the heating of a tricalcium silicate type Ca_3SiO_5. Beamline X7A was used to obtain data from a sample in a 0.3 mm quartz capillary tube using a Kr PSD, at a wavelength of 0.70313 Angstroms as determined by a CeO_2 standard. Rietica [9] was used for data analysis.

Results: Transitions $T_2 \rightarrow T_3 \rightarrow M_1$ were observed. Plots of lattice parameters a, b, c and the angles alpha, beta and gamma versus temperature were constructed from refinements in the triclinic P1bar crystal system. Higher temperature polymorph transitions were unable to be obtained due to instability in the quartz capillary tube.

Conclusions: The transition $T_2 \rightarrow T_3$ was successfully investigated. New structures for T_2, T_3 and M_1 modifications of tricalcium silicate were observed.

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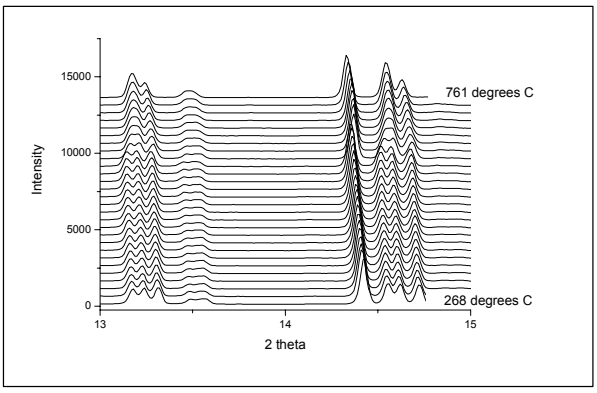

Figure 1: Synchrotron powder diffraction reflections of a tricalcium silicate sample at various temperatures